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RadHeat V1 User's Manual

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I. INTRODUCTION

RadHeat is a one dimensional finite difference heat transfer code that can determine the transient temperature evolution of layered targets in pulsed penetrating radiation environments. It makes use of energy dependent opacity and stopping data to model the volumetric deposition of any number of photon or ion spectra each incident at arbitrary angles. Convective and radiative boundary conditions are handled as well as the ability to impose any initial temperature profile. The heat diffusion equation is formulated implicitly to eliminate timestep dependent stability issues. Simulations are, therefore, able to achieve high fidelity during times of thermal activity and greater speed elsewhere. The prototypical physical situation simulated by RadHeat is illustrated in Figure 1.

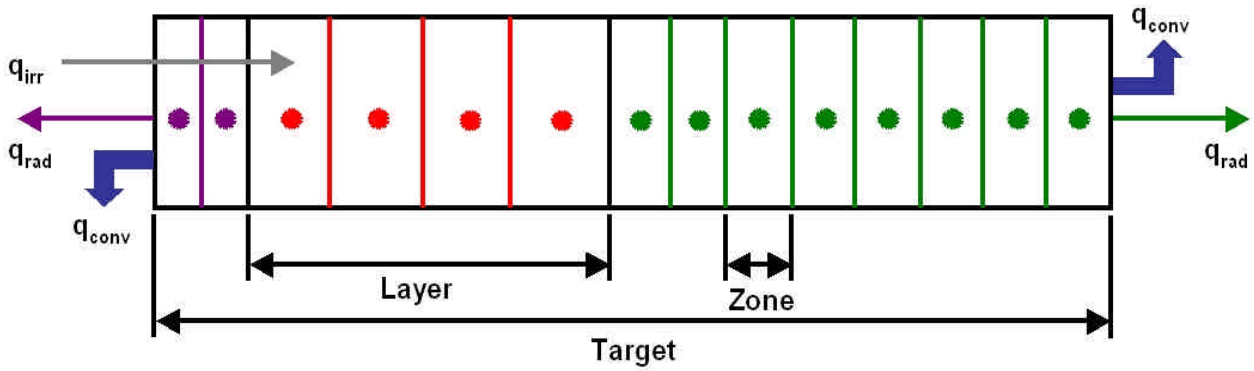

Fig. 1. A RadHeat target can have any number of layers composed of any number of materials (shown in different colors above). Heating by penetrating radiation (q_{irr}) from any number of ion or photon spectra each at arbitrary incidence angles can be determined and convective & radiative boundary conditions can be applied to the front and back target surfaces (q_{conv} and q_{rad}).

II. BACKGROUND

RadHeat was originally written to study the temperature response of tungsten-armored target-facing walls to the pulsed photon and ion radiation emanating from fusion microexplosions in future IFE power plants. RadHeat's implementation is quite general, though, and the code can be applied to a very broad range of problems. Anything from the heating of the Earth's crust on a warm summer day to the temperature rise in a mirror after a laser pulse could potentially be modeled. This manual was written to help new users learn how to run the code and introduce them to the simulation tools it provides.

III. SETTING UP A RADHEAT SIMULATION

The parameters that define a simulation for RadHeat are provided by various input files in the "/Setup/" folder located in the RadHeat installation directory. Among these are material property files, ion and photon spectra files, heating files, ion stopping files, and the master "Setup.inp" file. All of these follow fairly uniform formatting and naming conventions that will be illustrated below. These formatting conventions must be strictly adhered to or RadHeat will be unable to import the data contained in those

files. In the following pages, examples of input file text will be shown indented and in bold using the **Courier New** font. When finished editing any file, it is a good idea to hit "Ctrl-A" to highlight all the text in the file and look for unintentional invisible characters such as tabs or spaces. When these are adjacent to input strings RadHeat can become confused and will most likely hang looking for a file that does not exist.

The sections below discuss the input files and parameters needed by RadHeat to run a simulation. It is helpful to reference the sample data files provided with the distribution.

III.A. The "Setup.inp" file

The "Setup.inp" data file located in the "/Setup/" folder is the first input file referenced by RadHeat. It describes the geometry and other important parameters that define your model. It also determines what other data files will need to be referenced. The file is composed of various subsections described below. The appendix gives a complete example of a "Setup.inp" file.

III.A.1. Output File Identifier

This subsection of the "Setup.inp" file defines a string (which must be specified) that will be appended to RadHeat's output files. Besides automating the naming of these files, this allows you to run several instances of the program at once. Simply change the identifier string along with any other parameters and then once again run the RadHeat executable. Separate output files will be generated for this new run. The following example tells RadHeat to append the string "-Run2 - 11-24-04" to its output files.

```
**********************
OUTPUT FILE IDENTIFIER
**********************
-Run2 - 11-24-04
**********************
```

III.A.2. Import Heating Array

RadHeat has the ability to reuse information about zone heating from previous runs. This is useful because these computations are time consuming and one often wishes to conduct variation studies modifying only parameters that change during the timestepping portion of a simulation. Since zone heating from ion and photon spectra is calculated only once before timestepping and then applied identically each pulse, it is easy to read in a pre-calculated heating array rather than compose a new one each run. RadHeat automatically writes these heating arrays when appropriate, such as on runs where these arrays are not used and when at least one ion or photon spectra is specified. The example below shows how you would specify a heating file.

```
<
*************************
IMPORT HEATING ARRAY
HMF [dbl] =    2.0000e+00
*************************
HEATING-Run2 - 11-24-04.inp
*************************
```

This subsection (like all subsequent subsections in the “Setup.inp” file) has a delimiting symbol. Here, it is a “<”. In this example, RadHeat is asked to use the heating array stored in the file "HEATING-Run2 - 11-24-04.inp" which must be located in the "/Setup/Heating/" folder. Above the heating file name is the heating array magnitude factor HMF. The volumetric heating for each zone of an imported heating array will be scaled by this factor (2.0 in this case). If no heating array is needed, leave not gap between the two rows of asterisks where a name would otherwise go. HMF will be ignored.

III.A.3. Layering

The target layering specifications are handled in this subsection. Any number of layers can be specified with three parameters defining each layer. An example is given below.

```
&
*********************************
LAYERING
dL [m]          E[int]    Material
*********************************
1.0000e-06      10        Al.inp
9.0000e-06      9         Al.inp
9.0000e-05      9         W.inp
9.0000e-04      9         SiO2.inp
*********************************
```

The first parameter needed is “dL”, which is the thickness of the layer in meters. The second is an integer “E” representing the number of discrete elements you wish to break the layer into. The third parameter is a material file specification. RadHeat will read in material properties from a file with this name located in the ”/Setup/Properties/” folder. This subsection is delimited by the “&” symbol. Defined above is a target 1 mm thick made from aluminum (10 um), tungsten (90 um), and fused silica (0.9 mm). Multiple layers of the same material can be stacked to achieve any desired zoning.

III.A.4. Boundaries

This subsection defines for RadHeat the convective and radiative boundary conditions at the front and back of a target. The example below specifies a convective heat transfer coefficient at the front surface of 1000 W/(m^2K) and none at the back.

Both fluid temperatures are set at 300 K and the front and back blackbody radiation temperatures specified to be 273 K.

```
>
*******************************
BOUNDARIES
*******************************
TFf [K]          =    3.0000e+02
TBf [K]          =    3.0000e+02
hF [W/m^2/K]     =    1.0000e+03
hB [W/m^2/K]     =    0.0000e+00
TFr [K]          =    2.7300e+02
TBr [K]          =    2.7300e+02
*******************************
```

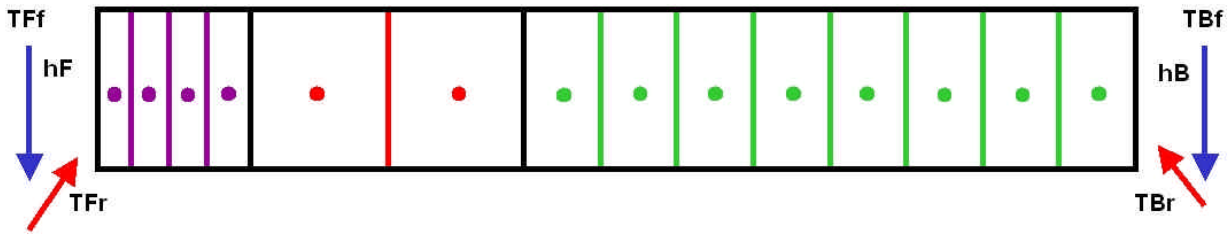

Fig. 2. Boundary condition parameters.

Figure 2 illustrates that (TFf) and (TBf) are the temperatures of coolant fluid at the front and back target surfaces, respectively, and (hF) and (hB) define the convective heat transfer coefficients for those fluids. (TFr) and (TBr) are the temperatures of the blackbody radiation incident on the front and back surface. All units for these quantities are defined in brackets to the right of the parameter name.

III.A.5. Initial Temperature Profile

The initial target temperature profile is specified with at least two points referencing normalized coordinates (s / W where W = total target thickness and a value 0 would represent the front of the target and 1 the back). Temperatures for each element are assigned based on a linear interpretation of the these points using their position in the target. Figure 3 shows a plot of the temperature profile called for in the example below across an arbitrary target.

```
~
*************************
INITIAL TEMP. PROFILE
s/W [0-1]      T [K]
*************************
0.0000e+00     3.0000e+02
2.5000e-01     5.0000e+02
7.5000e-01     6.0000e+02
1.0000e+00     3.0000e+02
*************************
```

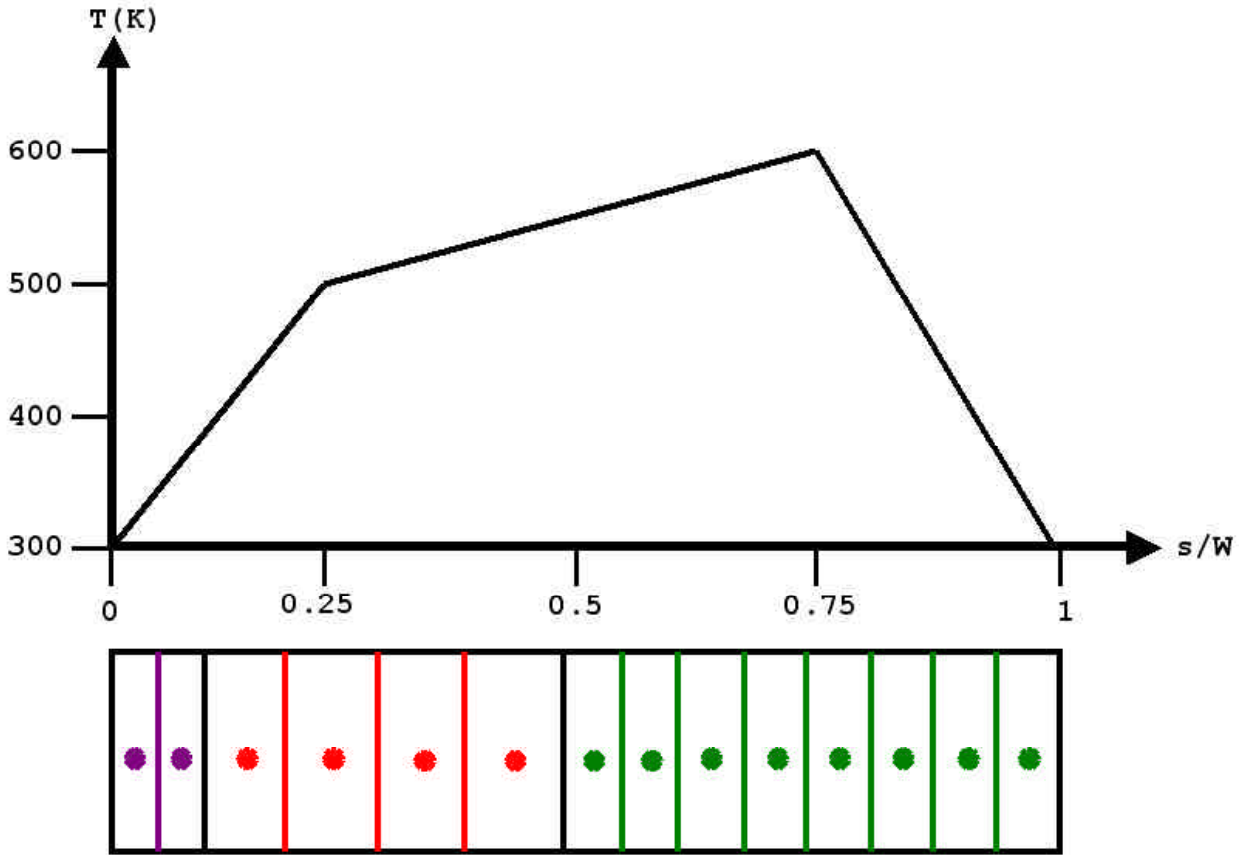

Fig. 3. Temperature profile across an arbitrary target specified by data points in example above.

III.A.6. Pulsing

This subsection defines the pulse frequency (f) and the number of pulses (P). The pulse frequency tells RadHeat how quickly to apply the selected photon and/or ion heating (e.g. once a second or ten times a second). The pulse number tells RadHeat how many times to do this (e.g. one time or one million times).

```
!
************************
PULSING
************************
f [1/s]   =    1.0000e+01
P [int]   =    10
************************
```

The example above specifies 10 pulses be applied to the target at a rate of 10 Hz.

III.A.7. Timesteps

This subsection tells RadHeat what size you want timesteps to be (determined from a linear interpolation of the numbers provided) over the course of a pulse period. On many occasions RadHeat will override the timestep magnitudes you specify to resolve critical events (such as the volumetric heating in an element changing), but for most of a pulse period your requested timesteps will apply. Any number of data points may be specified but points outside a pulse period will have no impact on the simulation. In the example below, from the start of each pulse until 10 ns afterward, the timestep magnitude will be 0.01 ns. As the pulse proceeds, the timesteps get larger until at the end of the pulse they are 0.1 ms.

```
@
************************
TIMESTEPS
t – p/f [s]    dt [s]
************************
0.0000e+00     1.0000e-11
1.0000e-08     1.0000e-11
1.0000e-07     3.0000e-10
3.0000e-07     3.0000e-09
3.0000e-06     3.0000e-09
5.0000e-06     3.0000e-08
1.0000e-05     5.0000e-08
1.0000e-04     3.0000e-07
1.0000e-03     3.0000e-06
1.0000e-02     3.0000e-05
1.0000e-01     1.0000e-04
************************
```

III.A.8. Photon Spectra

Here is where you specify the photon spectra you wish to apply. These need to be located in the “/Setup/Spectra/Photons/” folder. You can list as many or as few spectra as you wish (even a single spectrum several times). If you list none, leave no gap between the two rows of asterisks where the names of spectra would usually go.

```
%
*******************************************************************************
PHOTON SPECTRA
to[s]          Dt[s]          A[deg]         MF[dbl]        RF[int] Spectrum
*******************************************************************************
0.0000e+00     4.0000e-08     0.0000e+00     1.0000e+00     1       xapper.inp
*******************************************************************************
```

As can be seen, several parameters must be supplied along with the photon spectrum file name (“xapper.inp” in this case), “to” is the time at which the spectrum will be initiated, “Dt” is how long it will be applied, “A” is the spectrum’s off-normal incidence angle, and “MF” is a spectrum magnitude scaling factor similar to HMF described in section II.A.2. but only applied to this single spectrum. “RF” is a resolution factor that can be used to increase the number energy groups in a spectrum file. Increasing this factor judiciously is useful when only coarse grouping is supplied, which can lead to unrealistic temperature spikes from the sudden application of a large amount of volumetric heating. If a pre-calculated heating file is used, this section is ignored.

III.A.9. Ion Spectra

This subsection is identical to the “Photon Spectra” subsection described above except that it specifies ion spectra located in the “/Setup/Spectra/Ions/” folder.

```
?
*******************************************************************************
ION SPECTRA
to[s]          Dt[s]          A[deg]         MF[dbl]        RF[int] Spectrum
*******************************************************************************
0.0000e+00     1.0000e-10     0.0000e+00     1.0000e+00     1       Au197_D-154MJ-8m.inp
*******************************************************************************
```

III.A.10. Save Times

This subsection tells RadHeat when during each pulse you would like to save temperature profile data. This data will be saved at the same time for every pulse and be stored in the “RESULTS-Output File Identifier.dat” file located in the “/Results/” folder.

```
$
***********
SAVE TIMES
t - p/f [s]
***********
0.0000e+00
4.0000e-08
***********
```

The example above asks RadHeat to save a temperature profiles at the beginning of each pulse and 40 ns after that. “t” is the global time, “p” the pulse number (0,1,2,etc...) and “f” the pulse frequency. “t – p/f” is, therefore, the time since the beginning of the most recent pulse.

III.B. Material Property Files

Material property files specify properties needed to determine transient temperature profiles for layerd targets. These properties include melting temperature, thermal conductivity, specific heat, density, emissivity, and opacity. With the exception of opacities, which in RadHeat are dependent on photon energy, all material properties are temperature dependent. Values are assigned at each timestep in a simulation based on a linear interpolation of data provided in these files. The example below illustrates the formatting of a simple material property file for aluminum with constant properties.

```
**************************
MELTING TEMPERATURE
**************************
Tmelt [K] =    9.3347e+02
**************************
~
**************************
THERMAL CONDUCTIVITY
T [K]          k [W/m/K]
**************************
1.0000e+00     2.1800e+02
8.0000e+02     2.1800e+02
**************************
!
**************************
SPECIFIC HEAT
T [K]          c [J/kg/K]
**************************
2.0000e+02     7.9050e+02
6.0000e+02     7.9050e+02
**************************

@
**************************
DENSITY
T [K]          r [kg/m^3]
**************************
0.0000e+00     2.7000e+03
9.3347e+02     2.7000e+03
**************************
```

```
$
*************************
EMISSIVITY
T [K]          e [0-1]
*************************
0.0000e+00     0.0000e+00
9.3347e+02     0.0000e+00
*************************
%
*************************
OPACITIY
E [J]          g [1/m]
*************************
1.6020e-18     1.3132e+08
4.8060e-15     1.3132e+08
*************************
```

Obviously, these properties should not be used for a simulation where large temperature changes are expected and the above values would be invalid. A more realistic file for aluminum could be significantly larger with 10's or even 100's of points per property.

III.C. Photon Spectra Files

Photon spectra files have the format shown below. The data points provided define the spectrum's energy group boundaries and fluence densities. Photon spectra files are stored in the "/Setup/Spectra/Photons/" folder. Figure 4 shows a plot illustrating how photon spectra are interpreted by RadHeat.

```
*************************
E  [eV]        F[#/eV/m^2]
*************************
1.1250e+02     9.9422e+19
1.1350e+02     1.9422e+20
1.1450e+02     3.6455e+19
*************************
```

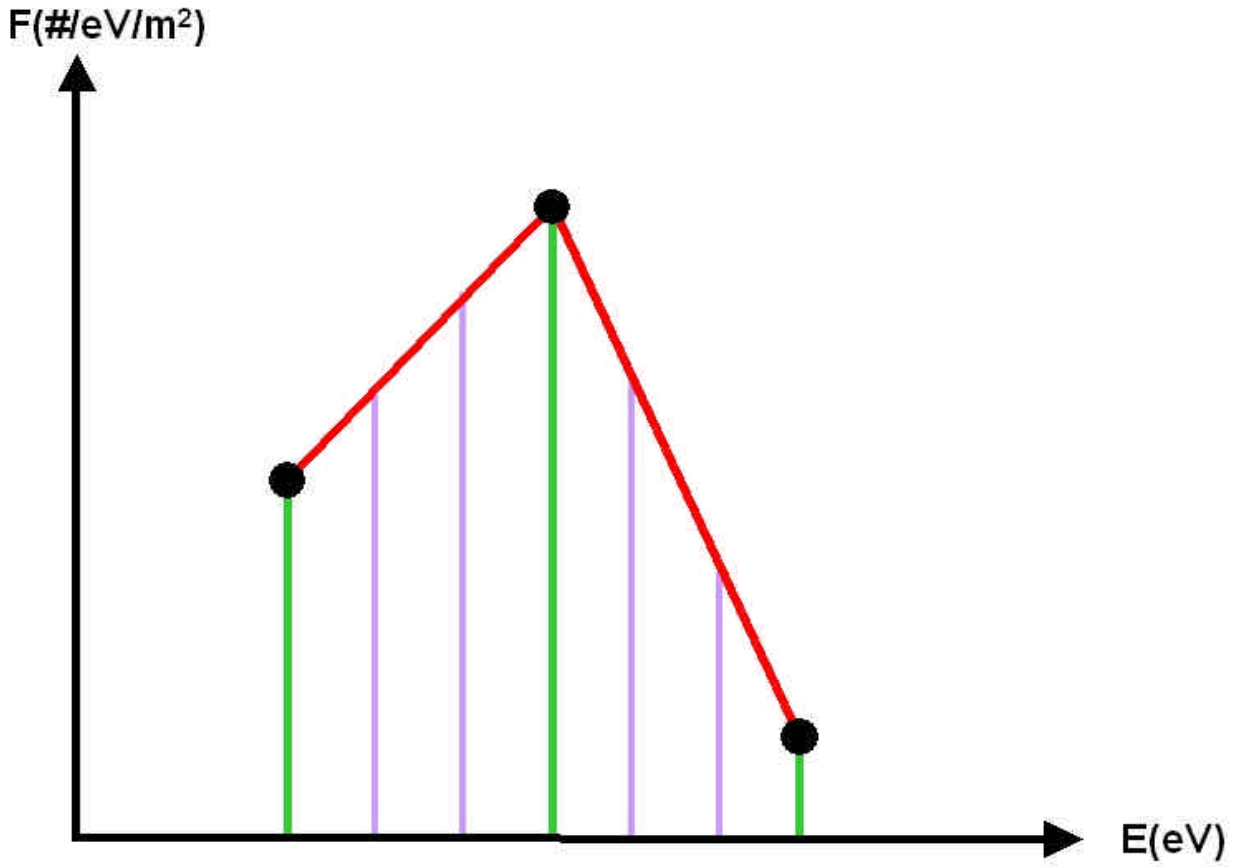

Fig. 4. A plot representing the data shown in the photon spectrum example above. The red lines connect the data points given and indicate the spectrum envelope, the green lines represent the group boundaries, and the purple lines indicate how each energy group would be broken up if a resolution factor (RF) of three were specified in the callout for this sepectrum in the "Setup.inp" file.

III.D. Ion Spectra Files

Ion spectra files are identical to photon spectra files except for their storage location ("Setup/Spectra/Ions/") and the addition of a parameter defining the mass of the ion.

```
**************************
m [amu] =      1.9700e+02
E  [eV]        F [#/eV/m^2]
**************************
1.8025e+00     6.2054e+18
3.2600e+00     6.2054e+18
8.6500e+00     1.2410e+19
**************************
```

A special naming scheme must be respected for ion spectra. The ion species is determined by the first part of the spectrum file name, which is delimted with either an

underscore ("_") or the period (".") symbol. This is used along with target layer material names to read in appropriate ion stopping files. What follows an underscore or period can be anything you desire to delineate different spectra of the same ion species. The naming scheme for stopping files will be covered in the next later section. If a pre-calculated heating file is used, this section is also ignored.

III.E. Stopping Files

Unlike material opacity data which (for a given material) can be used for all photon spectra, stopping data is specific to each ion species / material combination and all possible combinations must be available. Stopping files must be named according to a specific convention. The ion species name must precede the word "in" which must be followed by the material name. The template is "[ION SPECIES] in [MATERIAL].inp". The example below illustrates the formatting of a stopping file for Au197 (Gold) passing through aluminum (e.g. "Au197 in Al.sto").

```
**************************
E [eV]          w [eV/m]
**************************
1.0998E+00     8.1514E+09
1.2002E+00     8.5509E+09
1.3001E+00     9.0190E+09
1.4000E+00     9.4808E+09
1.4998E+00     9.9240E+09
1.5997E+00     1.0367E+10
1.7002E+00     1.0792E+10
1.8001E+00     1.1216E+10
**************************
```

On the left are numbers giving ion energy and on the right are the associated stopping powers. When an ion traverses a zone, the appropriate stopping power is interpolated from this data and used to determine how much thermal energy it will impart to the zone.

IV. RUNNING RADHEAT

Once the "Setup.inp" file is edited to describe your problem and all the necessary spectra, property, and stopping files are composed and placed in their proper directories, just double click on the "RadHeat.bat" file. This will start the "RadHeat.exe executable in low priority mode. For long runs this will ensure your computer is free to do other tasks. Depending on the nature of your problem, a run can take anywhere from a seconds to hours, or more.

V. READING RESULTS

RadHeat places simulation results are placed in the "/Results/" folder and titled "RESULTS+[identifier].out" file. This file includes a copy of the setup file for the run,

various parameters such as total photon and ion fluence, total absorbed fluence, and maximum zone heating, when appropriate. Also included are the locations of all zones and the temperature profiles for each zone at the times requested by in the “Save Times” subsection of the “Setup.inp” file. The first two columns in the temperature profile data give the global simulation time broken apart into two portions for your convenience. The first portion gives the time of the start of the pulse and the second column gives the inter-pulse time. To get the absolute time for a temperature profile, these two portions must be summed. All values are in seconds, meters, or Kelvin.

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APPENDIX

Shown below is the complete text of a RadHeat “Setup.inp” file. The output file indentifier is “-xapper” and a pre-calculated heating array is being used with no scaling (HMF = 1). The target is 1 cm thick and composed of 100 nm of aluminum on silicon dioxide. There is no convective cooling of the front or back surfaces and the blackbody radiation temperature is 300 K. The target is given a uniform initial temperature profile of 300 K. Twenty pulses each lasting 0.2 s are called for. Timesteps start small but ramp up as each pulse progresses. A photon spectrum is listed, but this entry is ignored by RadHeat because a heating file was already specified. No ions spectra are specified, though any entries would be similarly ignored. Temperature profiles will be saved at various times after each pulse.

```
*************************
OUTPUT FILE IDENTIFIER
*************************
-xapper
*************************
<
*************************
IMPORT HEATING ARRAY
HMF [dbl] =  1.0000e+00
*************************
HEATING-xapper.inp
*************************
&
*******************************
LAYERING
dL[m]        E[int] Material
*******************************
1.0000e-08   10     Al.inp
9.0000e-08   9      Al.inp
9.0000e-07   9      SiO2.inp
9.0000e-06   9      SiO2.inp
9.0000e-05   9      SiO2.inp
9.0000e-04   9      SiO2.inp
9.0000e-03   9      SiO2.inp
*******************************
```

```
>
**********************************
BOUNDARIES
**********************************
TFf [K]             =      3.0000e+02
TBf [K]             =      3.0000e+02
hF [W/m^2/K]  =      0.0000e+03
hB [W/m^2/K]  =      0.0000e+00
TFr [K]             =      3.0000e+02
TBr [K]             =      3.0000e+02
**********************************
~
*************************
INITIAL TEMP. PROFILE
s/W[0-1]     T[K]
*************************
0.0000e+00   3.0000e+02
1.0000e+00   3.0000e+02
*************************
!
*************************
PULSING
*************************
f [1/s]      =      5.0000e+00
P [int]      =      20
*************************
@
*************************
TIMESTEPS
t[s]         dt[s]
*************************
0.0000e+00   1.0000e-12
1.0000e-09   1.0000e-12
1.0000e-08   1.0000e-11
1.0000e-07   1.0000e-10
1.0000e-06   1.0000e-09
1.0000e-05   1.0000e-08
1.0000e-04   1.0000e-07
1.0000e-03   1.0000e-06
1.0000e-02   1.0000e-05
2.0000e-01   1.0000e-04
*************************
%
*****************************************************************************
PHOTON SPECTRA
to[s]        Dt[s]        A[deg]       MF[dbl]             RF[int]      Spectrum
*****************************************************************************
0.0000e+00   4.0000e-08   0.0000e+00   1.0000e+00   1      xapper.inp
*****************************************************************************
?
*****************************************************************************
ION SPECTRA
to[s]        Dt[s]        A[deg]       MF[dbl]             RF[int]      Spectrum
*****************************************************************************
*****************************************************************************
```

```
$
***********
SAVE TIMES
t - p/f [s]
***********
0.0000e+00
1.0000e-07
1.0000e-06
1.0000e-05
1.0000e-04
1.0000e-03
1.0000e-02
**********
```